**Minutes of the Research Directorate Meeting**
**Held on October 9, 2001, at Argonne National Laboratory**

**Attendees**:

APS:
S. Davey, R. Gerig, L. Keefe, B. Kustom, B. McDowell, T. Rauchas, G. Shenoy, S. Strasser, C. Vanni, and M. Vigliocco-Hagen

CAT Directors/Alternates:
E. Alp, R. Clarke, K. D'Amico, J. Chrzas, B. Fischetti, D. Hausermann, S. Heald, T. Irving, A. Joachimiak, D. Mills, J. Quintana, D. Robinson, G. Rosenbaum, C. Segre, J. Smith, J. Viccaro, R. Winans, and P. Zschack

**Routine Business**:

The minutes of the July 20, 2001, Research Directorate meeting were approved as written. Susan Strasser reviewed both the action items from the July meeting and the contents of the packets. The topic of cybersecurity was added to the meeting agenda.

**APS Update and Reports/Discussion Items**:

*APS Update*:
Gopal Shenoy reviewed recent results of the top-up run operations. The 2001 user survey conducted in August and September indicated that 98% of the users are pleased with top-up operations. The APS is the first user facility to implement this. Since the first beamline became operational in 1996, the increase in the user population has been dramatic. For FY2001, the APS hosted 1989 "unique users," at least 400 of whom were new to the APS. There has also been a significant growth in the Independent Investigator (II) area.

The APS is averaging 20 publications per beamline annually. Additionally, the number of protein structures solved at the APS deposited in the Protein Databank is also increasing. Since January 1, 2001, 20 *Physical Review Letters* (PRLs) have been published on work conducted at the APS. It is significant to note that a high school student interning at Carnegie has produced a PRL. Even though he was too young to work on the experiment hall floor, he carried out all of the data analysis.

*New APS ALD Appointment*:
J. Murray Gibson has been appointed as the new Associate Laboratory Director (ALD) for the APS. He has been at Argonne since 1998 as the Director of the Materials Science Division, specializing in nanoscience. His appointment will become effective on October 22, 2001.

*Cybersecurity Update:*
Bill McDowell briefed the group on the latest ANL Cybersecurity Firewall Program issues. An Argonne committee has been formed to review firewalls that are currently in place and will work with the CATs who may have specific concerns about the firewalls. Any major changes/modifications will have to go before the committee for its approval/disapproval. By November 9, the group will begin re-approving all "holes" in the network. The committee will be meeting every Thursday. Information about the program is available on the web. Links have been sent to CAT computer representatives.

*DOE/BES Program Review*:
Shenoy discussed the upcoming Department of Energy/Basic Energy Sciences (DOE/BES) Program Review of the APS that will be conducted October 16–18, 2001. Pedro Montano is organizing this review. The agenda includes overview presentations; scientific talks by APS users; a poster session; and discussions between the Review Committee members, APS CAT Directors, and APS Users Organization Steering Committee members. DOE will compose the final report based on summaries prepared by reviewers.

*PEB Review*:
Susan Strasser reviewed the PEB working agenda included in the packet of materials. This review is scheduled for October 24–26, 2001. Day one will focus on the HEX-CAT scientific proposal and the IMMW-CAT scientific case presentation of the bending-magnet line. Status reports from the GM/CA-, NE-, IXS-, Nano-, LS-, and COM-CATs are also on the agenda. Day two will consist of progress reviews of BESSRC-, DND-, and SRI-CATs.

*Survey Results*:
Denny Mills reviewed some of the highlights from the recent 2001 APS user survey. Topics covered in the survey included accelerator operations, administrative support, technical support, site amenities, and user support. The survey seemed to be well received, with 191 users responding and supplying the APS with 485 comments. More than 50% of the respondents were IIs. This type of survey will be continued in the future, probably at 18-month intervals to coincide with the Users Meetings. All survey results will be available on the web for review.

Mills also noted that the Decker lattice changes schedule is included in the packet materials. Any questions or concerns about the schedule should be directed to Denny Mills.

**CAT Updates**:

*BESSRC-CAT*:
As of January 1, 2002, Station 11-ID-D will be available for general users. This brings the total to five stations for general users: 12-ID-B, -C, -D, 12-BM, 11-ID-B, 11-ID-C,

and 11-ID-D. BESSRC-CAT has had 203 individual investigators representing 85 institutions (universities, industries, national labs and 10 foreign countries).

BESSRC-CAT is preparing for the APS review and the PEB review. Currently, BESSRC-CAT has 144 total publications, with 8 PRLs, one *Science*, one *PNAS*, and a *Journal of the American Chemical Society* article.

BESSRC-CAT is planning to hire a staff scientist to be in charge of the 12-ID beamline.

Finally, in beamline upgrades, a mirror that will allow pink beam in 12-ID will be installed in the near future.

*Bio-CAT*:
Two beamline scientist positions are open. Bio-CAT has made an offer (which will probably be accepted) to an experienced instrumentation scientist who will have primary responsibility for beamline developments as well as assist with user support. The other position is for a person to develop the biological XAFS user program.

Bio-CAT recently hosted the first outside macromolecular solution scattering users (Almo group, Albert Einstein University). It is expected that this activity will be a major part of the service user program.

The new 4k x 7k CCD detector is performing very well in preliminary SAXS applications. The single-photon detection capability and the high spatial resolution yielded excellent signal-to-noise ratio. Proof of principle time-resolved experiments have been done. A subcontract has been issued to W. Philip's group at Brandeis University for continued software developments to expand this capability.

A MIR structure of native rat tail collagen derived from data taken on the Bio-CAT beamline, the first such structure solution of its kind, will be appearing in *Structure* next month.

Bio-CAT has also been implementing flow systems for static and time-resolved XAFS.

*CARS-CAT*:

*CMC-CAT*:
CMC-CAT continues to commission instrumentation on its primary ID line. Most recently the SAXS apparatus in the C-station was completed to an extent where it can

now be used routinely in general user operation. With this new facility, CMC-CAT has 3 operational instruments on the ID line: a general-purpose 6-circle diffractometer, a horizontal liquid surface spectrometer and the SAXS apparatus. The beam transport on the BM line is close to completion; the PSS system has been installed and will be verified next month. End-station instrumentation for an EXAFS facility has been designed. First light on this beamline is expected early next year.

CMC-CAT has two permanent staff members and one Post Doc on site, Chitra Venkataraman, Thomas Gog, and Diego Casa, respectively. CMC-CAT has retained Rick Krakora from Sterling Engineering as a technician/draftsmen for another half year.

*COM-CAT*:

*DND-CAT:*

*GM/CA-CAT*:
Progress toward MOU:

- Submitting revised management plan and revised safety plan.
- Finalizing CDR for submission in about 1-1/2 weeks.
- Selected contractor for two separate contracts:
    - Design (Fixed Cost)
    - Build (Cost and Incentives)
    - Access to design exchange
- Established video conferencing capability to minimize travel.
    - Allows multi-session
    - Allows document transfer
    - Allows white board view
- In the process of posting positions for protein crystallographer, engineer, and systems manager.

*HP-CAT*:
<u>Enclosures and beam transport:</u>

- ID-A and ID-B: Construction complete.
- ID-C: Construction complete except for pneumatic door system.
- ID-D: 1/3 of structural assembly completed.
- But:

    - Construction now interrupted due to ANL's handling of the millwright's union industrial action.
- ID-A to ID-B beam transport:
    - Main branch: Installation in progress.
    - Side branch: Stands installed, beam tubes in transit.
- Electrical and PSS utilities installation in progress, the aim is to have ID-A, ID-B and the main branch transport line ready for the radiation tests in November.

Instrumentation:

- All the instrumentation / components for ID-A FOE have been designed and ordered. They are either at the fabrication or shipping stage. Deliveries started in July and will spread until the end of January 2002. Delivered so far:
    - 100W/400W aperture assembly.
    - High heat-load slits.
    - Stability blocks for branching monochromator.
    - ID-A pumping tee.
    - All ID-A support frames.
- And also:
    - Double-crystal monochromator: Final design review completed and approved. Construction in progress.
    - ID-A 100W thermal stop: Manufactured and tested. Ready for shipping.
    - ID-A radiation shutter for main branch: At detailed design stage.
- Experiment setups for ID-B are at the design stage. The experimental table design has been completed.
- An area detector will be ordered for delivery in February/March 2002.
- Vacuum, motor and beamline control, fluids supply RFQ stage.
- Mirrors (ID and BM): Quotation assessment stage.
- High-resolution monochromator and inelastic scattering spectrometer: Conceptual designs completed.
- Design work on all the other ID beamline elements in progress.
- BM beamline:
    - Cooled photon absorber for BM-C/D: Ready for shipment.
    - Radiation shutters for BM-B and BM-C/D: Ordered.

Support laboratories:

- General layout finalized, furniture delivered. Sample preparation equipment installed and being used for experiments on sectors 13, 3, and NSLS.
- Beamline equipment preparation laboratory being setup.

Instrument testing and experiments:

- Focusing Laue monochromator successfully tested at NSLS. Results under evaluation as this instrument is now planned for the BM beamline.
- The new cryostat has been successfully used at NSLS.
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Personnel:

- Markus Schwoerer has resigned effective October 1, 2001.

- One junior mechanical technician and one senior electrical/electronics technician started employment on August 6.
- Recruitment of another post doc in progress, with possible promotion to beamline scientist within six months.
- Searches: Two more beamline scientists with beamline construction/operation experience. Some interviews have already taken place.
- Other searches include one low-level control software programmer/administrator and one high-level control software programmer/administrator.
- Total number of full-time staff on October 1, 2001: eight. Consultant engineers and drafters: four, in the UK.

Budget:

- Spending profile on target.
- 2002 budget forecast being prepared.
- Total construction budget as per PDR WBS in complete agreement with project budget plan of 1997 despite many changes and increased project size (one extra fully equipped enclosure).

Other topics:

- Preliminary design report submitted in September and it is very close to a final.
- The Project Advisory Committee (PAC) has reviewed the PDR. A first meeting was held on October 10. No major problems were found, no changes need to be made, and the PAC was very impressed by the project and the PDR.

*IMCA-CAT*:

*IMMW-CAT*:

*MHATT-CAT*:

September saw the inauguration of Michigan's Frontiers of Physics Center: FOCUS (Frontiers in Optical, Coherent, and Ultrafast Science), the first of four major centers that were awarded in the first year of this new NSF program. An important component of the FOCUS Center is the use of ultrafast lasers for coherent control of matter. The femtosecond diffraction station at 7-ID-D is a key facility for this research; for example, MHATT-CAT's *Nature* report of ultrafast switching of x-ray beams exploiting a time-resolved version of the Borrmann effect.

Howard University's microbeam station (7-ID-B) is producing some of the highest resolution (200nm) white-beam Laue nano-indentation strain maps using pre-figured K-B mirror focusing. Another recent success at sector 7 is the use of a new technique for

direct structure determination of buried interfaces: coherent Bragg rod analysis (COBRA). This was developed in a collaboration between Michigan, Lucent, Hebrew University, and PNC-CAT. MHATT-CAT is using the COBRA technique to study heteroepitaxial oxides such as $Gd_2O_3$, $SrTiO_3$, and related ferroelectric oxides.

Michigan's Applied Physics department recently added David Reis to its faculty. Prof. Reis' research is in ultrafast diffraction physics and new pulsed x-ray sources. MHATT-CAT also added a third beamline scientist, Don Walko, who comes from the University of Illinois, via Northwestern and DND-CAT.

*MR-CAT*:

- Search still open for a new beamline scientist through the University of Florida.
- First working prototype of bent Laue analyzer and Ge high-energy beam cleaner. Finished commissioning on K-B microfocusing.
- MR-CAT has upgraded its XAFS scanning hardware to be able to perform full scans in as little as four seconds. This will be the routine operating mode.
- First IIs were at beamline in run 2001-3. Five experimenters have been invited, and MR-CAT expects to have five more during run 2001-4.

*MU-CAT*:

During this past cycle, MU-CAT hosted two different user groups on the primary ID line. These groups conducted resonant magnetic scattering and liquid surface scattering experiments. The bulk of the beam time was devoted to commissioning work postponed from the first year of operation. MU-CAT identified and eliminated a bizarre electromechanical resonance in the Kohzu monochromator due to a temperature-dependent coupling between a passive metal shield and the servo drive system for the primary axis.

Technical problems with the UHV surface scattering chamber precluded completion of experiments begun during the previous cycle.

Work continues to finish various technical issues left unresolved in the high-energy parallel beamline. MU-CAT hopes to be ready for CAT member users during the upcoming cycle.

The 6-BM line preliminary design report has been submitted. A requisition for the enclosures has been initiated.

*PNC-CAT*:

There have been no major changes with PNC-CAT since the last meeting. Personnel remain the same, and there is still no word on our operations funding proposal to DOE. The II program has begun, and several groups were hosted over the summer (in addition to the Canadian IIs that PNC-CAT has been hosting for the past two years).

On the ID beamline, routine operation of a new microtomography setup that gives a resolution better than two microns is being realized. Paper scientists at Weyerhauser are very interested in these capabilities and may become a contributing member of PNC-CAT. Most of the bugs in the femtosecond laser system have been worked out and it is ready to begin experiments.

The BM line is operating in unfocused mode and is being scheduled most of the time for CAT members and an occasional II (generally in conjunction with an ID run). A new vertically focusing mirror should arrive soon. Work has also begun on a sagittal bender for horizontal focusing. When this is commissioned (probably in mid 2002), plans call for declaring the BM line operational.

*SBC-CAT*:

*SER-CAT*:
ID beamline**:**

- All hutches have been validated.
- SER-CAT has monochromatic light in the experimental hutch with intensities measured at 12 keV ($1^{st}$ undulator harmonics) and at 15 keV ($3^{rd}$ undulator harmonics) being at the values calculated from undulator emission data.
- The end station instrumentation is close to complete installation.
- A prototype of the Bruker Proteum 300 detector has been received and is being integrated with the beamline and experimental control.
- The APS Metrology Lab has verified the high quality (as specified) of mirrors for the ID and BM fabricated by InSync.

BM beamline**:**

- Beneficial occupancy of all hutches has been realized.
- White beam transport has been received and is ready for installation.
- Support structures in hand will be installed as soon as floor plates have been grouted (awaiting availability of Tecknit technicians).
- Endstation instrumentation has been partly received and will be installed as soon as floor plates have been grouted.
- Mirror tank has been received.
- Hutches will be ready for validation in December but front end will not be installed until the April-May 2002 shutdown.

Personnel:
Job openings for sector manager, beamline scientist, and macromolecular crystallographer have been advertised in *Science*, at meetings, and posted at the APS. A number of applications have been received and evaluated; selection of sector manager is imminent.

*SGX-CAT*:

*SRI-CAT*:

*UNI-CAT*:
On October 9, Haydn Chen announced his resignation as UNI-CAT director. Chen has accepted a position at the City University of Hong Kong and has left the University of Illinois. The UNI-CAT Board of Governors (BOG) has decided that the UNI-CAT Management Plan should be rewritten to reflect the changeover from construction activities to operations. Tai Chiang (UIUC) was appointed Interim UNI-CAT Director and was charged with the rewriting. After approval is secured from both the BOG and the APS, Paul Zschack would be promoted to UNI-CAT director, and Chiang would serve as the chairman of the BOG.

In keeping with tradition, the UNI-CAT hosted a dinner event to dedicate the newest beamlines in sectors 33 and 34. The construction and installation activities are essentially completed on the ID beamline in sector 34 and the BM beamline in sector 33. UNI-CAT expects full-time commissioning experiments to begin during the next running period and hopes for full operations sometime early in 2002.

The first year of the UNI-CAT Independent Investigator Program was an unequivocal success. UNI-CAT provided 49 days of beam to IIs from eleven different groups. This accounted for 24% of all operations at 33-ID. Of the 27 proposals submitted for consideration in FY 2001, 22 were provided access to the UNI-CAT ID facility.